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6. AUTHOR(S) M. E. Zvanut					
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Alabama at Birmingham Department of Physics 310 Campbell Hall 1300 University Boulevard Birmingham, Alabama 35294-1170				8. PERFORMING ORGANIZATION REPORT NUMBER:	
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Charge State of Ge-Related Point Defects in Oxidized SiGe Alloys

M.E. Zvanut, PI  
University of Alabama at Birmingham  
Birmingham, AL 35294-1170

The first stage of this work focused on point defects in the oxide layer of oxidized SiGe alloys. An oxygen vacancy related defect, the Ge E' center, was found in oxides grown by thermal oxidation of SiGe. An annealing study showed that the center was unstable at temperatures just above room temperature (50° C). The results have been published in Applied Physics Letters 63, 3049 (1993) and, earlier, in a proceedings of the Materials Research Society (1992). The second part of the program addressed defects at the interface between SiGe and an overlying oxide. Both Si and Ge dangling bond centers, presumably resulting from dielectric-semiconductor mismatch, were shown to exist at the interface. The depth profile of the Ge center, which supports identification of this defect with an interface, was reported in a proceedings of the Materials Research Society (vol. 405, 1996). The significance of both the oxide and interfacial defects lies in their potential association with oxide hole traps and interface states, two entities which are known to hamper the success of pure Si-based devices.

SiO<sub>2</sub> films were thermally grown on 10%, 25%, and 40% Ge MBE grown SiGe layers. Both atmospheric and high pressure oxides were investigated. Metal oxide semiconductor capacitors formed with these structures were studied with the conventional 1 MHz capacitance voltage (CV) technique. However, as is often the case with Ge-based MOS capacitors, many competing processes complicate the interpretation of the CV curves; thus, further study using this technique was not pursued. Rather, the defects in both the oxide films and at the interface were studied using electron paramagnetic resonance spectroscopy (EPR). The technique addresses the structure and density of atomic level defects.

EPR centers in the films reported prior to this grant-supported research were activated by 10 keV x-rays. Because similar center have been detected in bulk silica subjected to ultraviolet irradiation, work for the grant concentrated on detecting the Ge E' center as well as two other Ge-related oxide centers after illumination in the near ultraviolet (200-300 nm). Neither a 50 W D<sub>2</sub> lamp nor a frequency tripled Nd:YAG laser produced useful results. Presumably the former provided insufficient power. In the latter case, the threshold for damage in the UV pulse was lower than the threshold for point defect generation; thus, we succeeded only in ablating the oxide surface. Although we were unable to reveal any new defect centers in the oxide films, the work did reveal the first observation of the Ge E' center in thermally oxidized SiGe films.

Although Ge-incorporated oxide films may have relevance in micro-optical applications, such layers appear to be unacceptable as gate dielectrics in device applications.

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Rather, work focuses on mating pure  $\text{SiO}_2$  and alternative dielectrics to the SiGe alloy system. In these systems as well as in thermally grown oxide structures, broken or strained bonds at the interface between the alloy and overlying layer are a common problem. Thus, the latter portion of our work has focused on the interfacial region. Here, we have studied both the Si and Ge dangling bond centers. Although, we have not yet observed the centers in the technologically relevant planar SiGe structures, we have shown that such defects may exist by identifying them in SiGe/oxide precipitate systems. Samples consisting of a SiGe/oxide/SiGe sandwich on a Si substrate were formed by oxygen implantation into MBE grown  $\text{Si}_x\text{Ge}_{1-x}$  layers. After annealing the samples in an inert environment at  $900^\circ\text{C}$ , the spectrum shown in figure 1a was obtained. Both the Ge dangling bond (SG1) and Si dangling bond ( $\text{P}_b$ ) signals are identified. To verify that these signals originate at the oxide precipitate-SiGe interface, a depth profile was obtained. EPR measurements of the samples after sequential etches in KOH and HF revealed that the density of both centers decreased as the portion of the sample containing the oxide precipitates was removed (figs. 1b, 1c, and 1d). Figure 2 shows the depth profile determined by measuring the etch step with a surface profilometer and the defect signal with EPR. The oxide precipitates are located in regions I and III. Clearly, the defects are not located at planar interfacial regions or in the oxide bulk, rather they appear to be associated with the oxide precipitate-SiGe interface. Details of this work appear in the accompanying reprint.

The equipment and samples necessary to study the interfacial defects on a planar SiGe/oxide interface have been assembled during the course of this award. The key to observing the centers at planar interfaces is the elimination of impurities, particularly hydrogen, from the interface. This is accomplished by annealing the samples in a dry environment. We have built a double-walled furnace capable of 0.5ppm moisture levels at  $1000^\circ\text{C}$ . Roughened Si samples annealed in this furnace produced two types of Si dangling bond centers, the well-studied  $\text{P}_{b0}$  and  $\text{P}_{b1}$  centers. Earlier studies on Si show that in order to maximize detection capability, samples should be quenched to room temperature in a dry environment. The modification necessary for this will be implemented this summer.

The primary result of this work is confirmation that the defect observed in O implanted SiGe is related to the interface between the SiGe and oxide. The center was shown to exhibit properties similar to the interfacial dangling bond observed in Si systems. Thus, the electrically deleterious Si interfacial dangling bond center present in Si/ $\text{SiO}_2$  structures has a Ge analogue in SiGe. This opens the door to the possible existence of a family of interface centers residing in different double-layer semiconductor-insulator structures. Other wide band-gap semiconductors such as SiC and GaN may exhibit similar interfacial dangling bond centers. Given the well-established role of dangling bonds in Si systems, these centers should be thoroughly addressed in the alternative semiconductor-dielectric systems.

### Personnel Involved in this Project

Two graduate students and one undergraduate participated, at various times, in this project. The first graduate student set-up the UV studies of the oxide films. The second pursued the interfacial centers and performed the etching studies. The undergraduate concentrated on writing analysis programs to address the electrical quality of the oxide/SiGe system. An interface state density analysis program was written and has been used in analysis of non-Ge based systems such as hydrogenated SiO<sub>2</sub>/Si structures.

### Samples/Collaborators:

SiGe layers were grown in the MBE facility at NRL under the direction of Dr. P. Thompson.

Oxide layers:

- atmospheric oxidation performed in the nanofabrication facility at NRL
- high pressure oxidation performed at Brown University under the direction of Dr. D. Paine

O implantation - samples received through NRL

X-TEM - depth profile obtained under this contract was determined by comparison of a cross sectional TEM micrograph obtained by Dr. M. Twigg, NRL.

### Publications in print during the tenure of this Grant

Patricia J. Macfarlane\*, M.E. Zvanut, W.E. Carlos, M.E. Twigg, and P.E. Thompson, "Ge-Related Interfacial Defects in SiGe Alloy Structures" in Surface, Interface, and Stress Effects in Electronic Material Nanostructures edited by S.M. Prokes, K.L. Wang, R.C. Cammarata, and A. Christou (Mater. Res. Soc. 405, Pittsburg, Pa 1996).

M.E. Zvanut, W.E. Carlos, D. C. Paine, and C. Caragianis, "Atomic structure of Ge-related point defects in Ge-incorporated oxide films", Appl. Phys. Lett. 63, 3049 (1993).

### Presentations made during the tenure of this Grant

Patricia J. Macfarlane\*, M.E. Zvanut, W.E. Carlos, and M.E. Twigg, "Ge-Related Interfacial Defects in SiGe Alloy Structures", Materials Research Society Meeting, Boston MA, December 1995.

M.E. Zvanut and Patricia J. Macfarlane\*, "The SG1 Defect: A Ge Dangling Bond in Oxygen Implanted SiGe", Rocky Mountain Conference on Analytical Chemistry, Denver CO, July 1995.

\*supported by AASERT

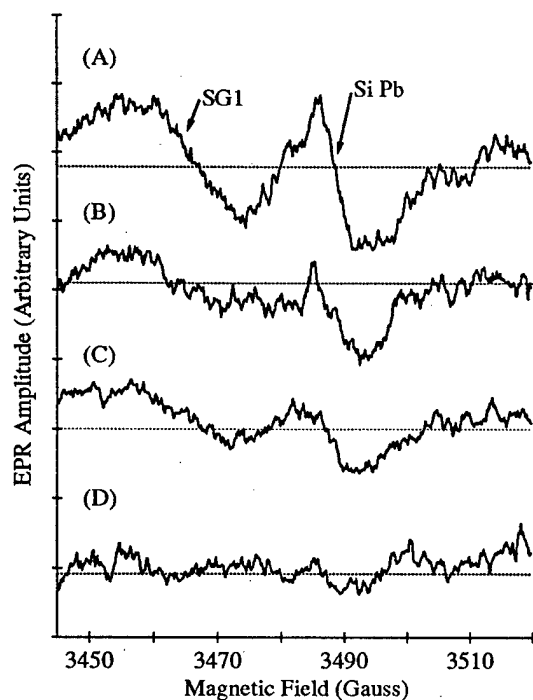


Figure 1. EPR spectra obtained after:  
 (A) growth of 40 nm anchor oxide  
 (B) 15 min KOH etch  
 (C) 20 min KOH and 2.75 min HF etch  
 (D) additional 90 min KOH etch

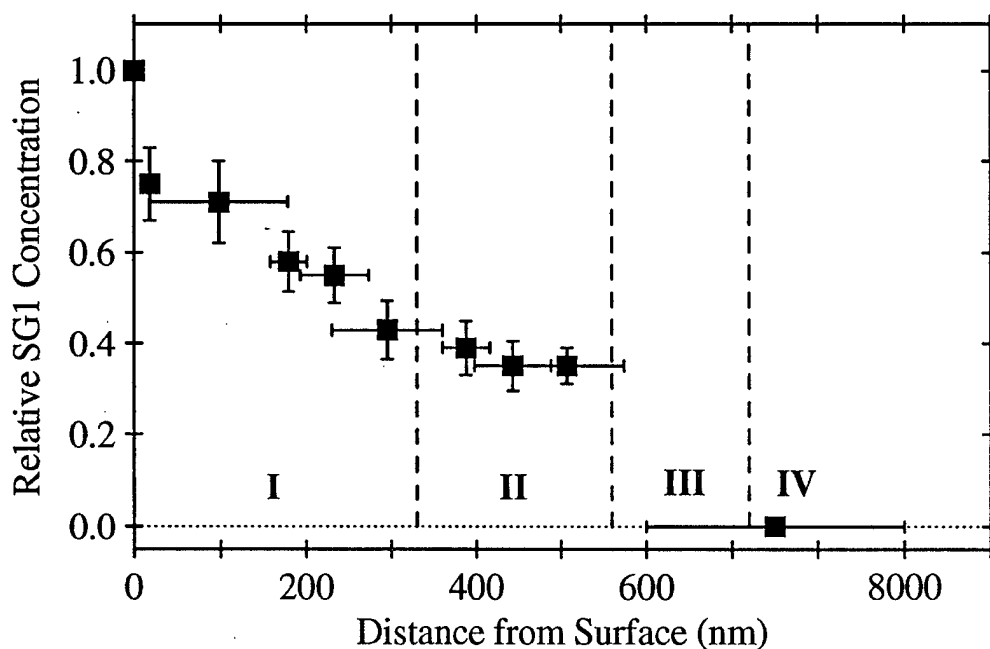


Figure 2. Depth profile for SG1 center; y-axis represents the original surface of the top SiGe layer. I, crystalline SiGe; II, buried oxide; III, damaged SiGe; IV, unimplanted SiGe